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320. CALCULATIONS OF NLO-PROPERTIES OF DONOR-ACCEPTOR DIPHENYLSILANES

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Highly polar molecules in a polymer matrix are suitable for second harmonics generation devices since they orient on high voltage poling above T_g . Silicon-based donor-acceptor (DA-) compounds have potential since they are transparent in the visible spectrum, and have large dipoles and moderate values of the first hyperpolarizability β . Our study (synthesis, optical characterization and calculations) focuses on DA-diphenyldisilanes, and their incorporation into polymer. The quantum chemical calculations (semi-empirical and *ab initio*, finite-field and sum-over-states (SOS)), are compared mutually and with experimental results. The SOS method yields useful predictions for β . Acceptors containing the sulfonyl group prove to be efficient and retain transparency for the DA-compound. Charge distributions of ground and excited states show that the silicon chain is a charge buffer and a weak transmitter.

321. SYNTHESIS AND PROPERTIES OF 2ND-ORDER NLO-ACTIVE POLYSTYRENE AND AMYLOSE BASED MATERIALS.

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Second order non-linear optical effects might lead to novel applications as integrated electro-optic devices. Polymers functionalised with NLO-active groups seem to have good properties for these applications. We have synthesized a polystyrene based NLO-material that can be poled by corona discharge or contact poling to give a very good ordering ($\Phi=0.45$). The r_{33} value directly after poling was 12.9 pm/V. The bleachability of the material gives the possibility to make channel waveguides by exposing the material to UV-light through photomasks. Another way to order macroscopic systems is the Langmuir-Blodgett (LB) technique. We have synthesized an amylose derivative with covalently bound NLO-active groups. This material forms stable monolayers.

322. SECOND HARMONIC GENERATION FROM LB FILMS OF POLY(ISOCYANIDE)S.

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In this study poly(isocyanide)s are used for Langmuir-Blodgett film formation. These rigid rod helical polymers can be obtained either racemic or optical pure. The polymers which contain azobenzene based side groups with a dialkylamino end group do not form stable layers. However mixing these polymers with amylose-ester derivatives resulted in stable transferable films. Up to at least 100 layers could be deposited, Y-type, with constant transfer ratios. Thicknesses and refractive indices were measured by means of ellipsometry. The monolayer thickness showed to scale linearly with the base mole fraction poly(isocyanide) in the mixed film. Second Harmonic Generation (SHG) from multilayers was measured and the second harmonic signal showed higher in case of the polymer obtained from polymerization of a chiral isocyanide.

323. Silicon-Based Donor-Acceptor Compounds in a Polymer Matrix. Diny Hissink, Henk J. Bolink, Jan-Willem Eshuis, George G. Malliaras and Georges Hadziioannou, Department of Polymer Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

For many applications involving nonlinear optical phenomena (e.g. frequency doubling) transparency in the visible spectrum is a requirement. We have